Effect of Spin-Flip Scattering on Electrical Transport in Magnetic Tunnel Junctions

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Abstract

By means of the nonequilibrium Green function technique, the effect of spin-flip scatterings on the spin-dependent electrical transport in ferromagnet-insulator-ferromagnet (FM-I-FM) tunnel junctions is investigated. It is shown that Jullière′s formula for the tunnel conductance must be modified when including the contribution from the spin-flip scatterings. It is found that the spin-flip scatterings could lead to an angular shift of the tunnel conductance, giving rise to the junction resistance not being the largest when the orientations of magnetizations in the two FM electrodes are antiparallel, which may offer an alternative explanation for such a phenomenon observed previously in experiments in some FM-I-FM junctions. The spin-flip assisted tunneling is also observed.

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Spin-dependent electrical transport in magnetic tunnel junctions has received much attention both theoretically and experimentally in recent years (see e.g. Refs. [1] for review). A new field dubbed as *spintronics* (i.e. spin-based electronics) is emerging. Among others one of the simplest devices in spintronics would be a ferromagnet-insulator-ferromagnet (FM-I-FM) structure which is comprised of two ferromagnetic electrodes separated by an insulator thin film. In 1975 Jullière made the first observation of spin-polarized electrons tunneling through an insulator film into a ferromagnetic metal film, and clearly observed 14% tunnel magnetoresistance (TMR) for Fe/Ge/Co junctions at 4.2 K [2]. In 1995, Moodera et al made a breakthrough that they observed over a 10% TMR for a $Co/Al_2O_3/Ni_{80}Fe_{20}$ junction reproducibly at room temperature [3]. Since then, there are a variety of works toward enhancing TMR in magnetic tunnel junctions, and the TMR $> 30\%$ has been obtained at room temperature [1]. On the other hand, to understand the spin-polarized tunneling results for FM-I-FM junctions, people usually invoke the model based on a classical tunneling theory proposed by Jullière [2], in which spins of electrons during tunneling are supposed to be conserved, namely, the tunneling of spin-up and spin-down electrons are two quite independent processes, and spin-flip scatterings are neglected. Though Jullière's two-current model can interpret well some experimental results qualitatively, it still faces to difficulties for more complex situations. Actually, in some experiments spin conservation no longer holds, and the spin-flip scattering may take effect on the transport properties. There has been a number of experiments [1,4] showing that TMR can be very various for different barriers, and the inverse TMR can even occur, namely, the resistance when the orientations of magnetizations of the two ferromagnets are parallel, is larger than that of antiparallel orientations. It appears that the spin-flip scatterings might not be ignored in these situations. Recently, Vedyayev et al investigated a model including impurities in the middle of the barrier, and considered both cases of spin conserving scattering and spin-flip scattering [5]. Besides, Jaffrès et al measured the angular dependence of the TMR for transition-metal based junctions, and observed that the angular response is beyond the simple cosine shape [6].

In this paper, based on a microscopic model and using the nonequilibrium Green function technique we shall give a more general expression of the angular dependence of the TMR for FM-I-FM junctions by including the effect of spin-flip scatterings. It is found that the effect of spin-flip scatterings gives rise to a correction to the formula of the usual tunnel conductance. Specifically, we have found that the spin-flip scattering induces a phase shift, leading to the tunnel conductance not to be the smallest when the magnetizations of the two FM electrodes are antiparallel, which may provide an alternative explanation for the previously experimental observation of the angular shift in some FM-I-FM tunnel junctions. In addition, it has been shown that the spin-flip scattering could also lead to the inverse TMR effect under certain conditions though it is not the only factor, and the spin-flip assisted tunneling is also observed.

Let us consider a magnetic tunnel junction consisting of two ferromagnetic films separated by an insulator thin film. A steady bias voltage is applied to the junction. The relative orientation of magnetizations in the two ferromagnets is characterized by the angle θ. The Hamiltonian of the system reads

$$H = H_L + H_R + H_T, \tag{1}$$

with

$$
\begin{aligned}
H_L &= \sum_{k\sigma} \varepsilon_{k\sigma}^L a_{k\sigma}^\dagger a_{k\sigma}, \\
H_R &= \sum_{q\sigma} [(\varepsilon_R(\mathbf{q}) - \sigma M_2 \cos\theta) c_{q\sigma}^\dagger c_{q\sigma} - M_2 \sin\theta c_{q\sigma}^\dagger c_{q\overline{\sigma}}], \\
H_T &= \sum_{kq\sigma\sigma'} [T_{kq}^{\sigma\sigma'} a_{k\sigma}^\dagger c_{q\sigma'} + T_{kq}^{\sigma\sigma'*} c_{q\sigma'}^\dagger a_{k\sigma}],
\end{aligned}
$$

where $a_{k\sigma}$ and $c_{k\sigma}$ are annihilation operators of electrons with momentum k and spin σ ($=\pm 1$) in the left and right ferromagnets, respectively, $\varepsilon_{k\sigma}^L = \varepsilon_L(\mathbf{k}) - eV - \sigma M_1$, $M_1 = \frac{g\mu_B h_L}{2}$, $M_2 = \frac{g\mu_B h_R}{2}$, g is Landé factor, μ_B is Bohr magneton, $h_{L(R)}$ is the molecular field of the left (right) ferromagnet, $\varepsilon_{L(R)}(\mathbf{k})$ is the single-particle dispersion of the left (right) FM electrode, V is the applied bias voltage, $T_{kq}^{\sigma\sigma'}$ denotes the spin and momentum dependent tunneling amplitude through the insulating barrier. Note that the spin-flip scattering is included in H_T when $\sigma' = \bar{\sigma} = -\sigma$. It is this term that violates the spin conservation in the tunneling process. By performing the $u - v$ transformation, $c_{q\sigma} = \cos\frac{\theta}{2} b_{q\sigma} - \sigma \sin\frac{\theta}{2} b_{q\overline{\sigma}}$, $c_{q\sigma}^\dagger = \cos\frac{\theta}{2} b_{q\sigma}^\dagger - \sigma \sin\frac{\theta}{2} b_{q\overline{\sigma}}^\dagger$, H_R becomes $H_R = \sum_{q\sigma} \varepsilon_{q\sigma}^R b_{q\sigma}^\dagger b_{q\sigma}$, with $\varepsilon_{q\sigma}^R = \varepsilon_R(\mathbf{q}) - \sigma M_2$, and H_T becomes $H_T = \sum_{kq\sigma\sigma'} T_{kq}^{\sigma\sigma'} (\cos\frac{\theta}{2} a_{k\sigma}^\dagger b_{q\sigma'} - \sigma' \sin\frac{\theta}{2} a_{k\sigma}^\dagger b_{q\overline{\sigma'}}) + h.c.$. The tunneling current has the form of

$$
I_L(V) = e\left\langle \dot{N}_L \right\rangle = -\frac{2e}{\hbar} \operatorname{Re} \sum_{kq} Tr_\sigma \{ \mathbf{\Omega}_{kq} \cdot \mathbf{G}_{kq}^<(t,\ t) \}, \tag{2}
$$

where $\mathbf{\Omega}_{kq} = \mathbf{T}_{kq} \cdot \mathbf{R}$ with $\mathbf{T}_{kq} = \begin{pmatrix} T_{kq}^{\uparrow\uparrow} & T_{kq}^{\uparrow\downarrow} \\ T_{kq}^{\downarrow\uparrow} & T_{kq}^{\downarrow\downarrow} \end{pmatrix}$ and $\mathbf{R} = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$, and Tr_σ stands for the trace of matrix taking over the spin space. The lesser Green function, $\mathbf{G}_{kq}^<(t,\ t')$, is defined in a steady state as

$$
\mathbf{G}_{kq}^<(t -\ t') = \begin{pmatrix} G_{kq}^{\uparrow\uparrow,<}(t-t') & G_{kq}^{\downarrow\uparrow,<}(t-t') \\ G_{kq}^{\uparrow\downarrow,<}(t-t') & G_{kq}^{\downarrow\downarrow,<}(t-t') \end{pmatrix}, \tag{3}
$$

with $G_{kq}^{\sigma\sigma',<}(t-t') \equiv i\left\langle a_{k\sigma}^\dagger(t') b_{q\sigma'}(t) \right\rangle$. To obtain the lesser Green function, one needs to introduce a time-ordered Green function $\mathbf{G}_{qk}^t$ as

$$
\mathbf{G}_{qk}^t(t-t') = \begin{pmatrix} G_{qk}^{\uparrow\uparrow,t}(t-t') & G_{qk}^{\uparrow\downarrow,t}(t-t') \\ G_{qk}^{\downarrow\uparrow,t}(t-t') & G_{qk}^{\downarrow\downarrow,t}(t-t') \end{pmatrix}, \tag{4}
$$

with $G_{qk}^{\sigma\sigma',t}(t-t') \equiv -i\left\langle T\{ b_{q\sigma}(t) a_{k\sigma'}^\dagger(t') \} \right\rangle$. By using the equation of motion, we get

$$
\mathbf{G}_{qk}^t(\varepsilon) = \sum_{q'} \mathbf{F}_{qq'}^t(\varepsilon) \mathbf{\Omega}_{kq'}^\dagger \mathbf{g}_{kL}^t(\varepsilon), \tag{5}
$$

with

$$
\mathbf{F}_{qq'}^t(\varepsilon) = \mathbf{g}_{q'R}^t(\varepsilon)\delta_{qq'} + \sum_{k'} \mathbf{G}_{qk'}^t(\varepsilon) \mathbf{\Omega}_{k'q'} \mathbf{g}_{q'R}^t(\varepsilon), \tag{6}
$$

where the use has been made of the Fourier transform of the time-ordered Green function $\mathbf{G}^t_{qk}(\varepsilon) = \int dte^{i\varepsilon(t-t')}\mathbf{G}^t_{qk}(t-t')$, and $\mathbf{g}^t_{kL}(\varepsilon)$, $\mathbf{g}^t_{q'R}(\varepsilon)$ are the time-ordered Green function of the left and right FM electrodes for the uncoupled system, respectively. By applying the Langreth theorem [9] to Eq.(5), we get

$$\mathbf{G}^<_{kq}(\varepsilon) = \sum_{q'}[\mathbf{F}^r_{qq'}(\varepsilon)\mathbf{\Omega}^\dagger_{kq'}\mathbf{g}^<_{kL}(\varepsilon) + \mathbf{F}^<_{qq'}(\varepsilon)\mathbf{\Omega}^\dagger_{kq'}\mathbf{g}^a_{kL}(\varepsilon)], \tag{7}$$

where the superscript "r(a)" denotes the "retarded (advanced)" Green function. The tunneling current becomes

$$I_L(V) = -\frac{2e}{\hbar}\int\frac{d\varepsilon}{2\pi}\mathrm{Re}(\sum_{k,q,q'}\{Tr_\sigma(\mathbf{\Omega}_{kq}[\mathbf{F}^r_{qq'}(\varepsilon)\mathbf{\Omega}^\dagger_{kq'}\mathbf{g}^<_{kL}(\varepsilon) + \mathbf{F}^<_{qq'}(\varepsilon)\mathbf{\Omega}^\dagger_{kq'}\mathbf{g}^a_{kL}(\varepsilon)])\}). \tag{8}$$

To get useful analytical result we may assume for simplicity that the tunneling amplitude $\mathbf{T}_{kq}$ is independent of the momentum like the conventional consideration [1], but depends on spin. This suggests that apart from inclusion of the spin-flip scattering we have supposed that the tunneling amplitude of electrons for the spin-up channel differs from that of the spin-down channel. As a result, $\mathbf{T}_{kq}$ becomes $\mathbf{T} = (\begin{matrix} T_1 & T_2 \\ T_3 & T_4 \end{matrix})$. In addition, the elements of $\mathbf{T}$ are assumed to be real. Up to the first-order approximation to the Green function $\mathbf{F}^t_{qq'}(\varepsilon)$, we get

$$I_L(V) = \frac{2e}{\hbar}\mathrm{Re}\int\frac{d\varepsilon}{2\pi}[f(\varepsilon) - f(\varepsilon + eV)]Tr_\sigma[\mathbf{T}_{eff}(\varepsilon, V)], \tag{9}$$

where $f(\varepsilon)$ is the Fermi function,

$$\mathbf{T}_{eff}(\varepsilon, V) = 2\pi^2\mathbf{T}\cdot\mathbf{R}\cdot\mathbf{D}_R(\varepsilon)\cdot\mathbf{R}^\dagger\cdot\mathbf{T}^\dagger\cdot\mathbf{D}_L(\varepsilon + eV), \tag{10}$$

and $\mathbf{D}_{L(R)}(\varepsilon)$ is a 2×2 diagonal matrix with two nonzero elements being the corresponding density of states (DOS) of electrons with spin up and down in the left (right) ferromagnet. For a small bias voltage V, we obtain the tunneling conductance

$$G = \frac{2e^2}{h}T_{eff}, \tag{11}$$

where $T_{eff} = Tr_\sigma[\mathrm{Re}(\mathbf{T}_{eff}(\varepsilon_F, V = 0))]$, and ε_F is the Fermi energy. In comparison to the Landauer-Büttiker formula, one may find that T_{eff} can be regarded as an effective tunneling transmission coefficient which includes the contribution from spin-flip scatterings. Eq. (11) can be explicitly rewritten as

$$G = G_0[1 + P_2\sqrt{P_1^2 + P_3^2}\cos(\theta - \theta_f)], \tag{12}$$

where $G_0 = \frac{\pi e^2}{2\hbar}[(T_1^2 + T_2^2)D_{L\uparrow} + (T_3^2 + T_4^2)D_{L\downarrow}](D_{R\uparrow} + D_{R\downarrow})$, $P_1 = \frac{(T_1^2 - T_2^2)D_{L\uparrow} - (T_4^2 - T_3^2)D_{L\downarrow}}{(T_1^2 + T_2^2)D_{L\uparrow} + (T_3^2 + T_4^2)D_{L\downarrow}}$, $P_2 = \frac{D_{R\uparrow} - D_{R\downarrow}}{D_{R\uparrow} + D_{R\downarrow}}$, $P_3 = \frac{2(T_1T_2D_{L\uparrow} + T_3T_4D_{L\downarrow})}{(T_1^2 + T_2^2)D_{L\uparrow} + (T_3^2 + T_4^2)D_{L\downarrow}}$, $\tan\theta_f = \frac{P_3}{P_1}$, $D_{L\uparrow} = D_L(\varepsilon + M_1 + eV)$, $D_{L\downarrow} = D_L(\varepsilon - M_1 + eV)$, $D_{R\uparrow} = D_R(\varepsilon + M_2)$, $D_{R\downarrow} = D_R(\varepsilon - M_2)$, and $D_{L(R)}$ is the DOS of electrons in the left (right) ferromagnet. One may observe that there is an angular shift induced by the spin-flip scatterings, as to be discussed below.

Now let us look at the angular dependence of the conductance G. When the spin-flip scattering is neglected, i.e. $T_2 = T_3 = 0$, and if we further assume $T_1 = T_4$, we recover the conventional expression for the conductance $G = \bar{G}_0(1 + \bar{P}_1 P_2 \cos\theta)$, which is familiar in literature [1,7], where $\bar{G}_0 = \frac{\pi e^2}{2\hbar} T_1^2 (D_{L\uparrow} + D_{L\downarrow})(D_{R\uparrow} + D_{R\downarrow})$, and $\bar{P}_1 = \frac{D_{L\uparrow} - D_{L\downarrow}}{D_{L\uparrow} + D_{L\downarrow}}$ is the usual polarization of the left ferromagnet, and $P_3 = 0$. When $T_2 = T_3 = 0$ but $T_1 \neq T_4$, which implies that even if the spin-flip scattering is ignored, but the tunneling amplitude of electrons for the spin-up channel is different from that for the spin-down channel, we can also get in this situation an expression

$$G = G_0'(1 + P_1' P_2 \cos\theta), \tag{13}$$

where $G_0' = \frac{\pi e^2}{2\hbar}(T_1^2 D_{L\uparrow} + T_4^2 D_{L\downarrow})(D_{R\uparrow} + D_{R\downarrow})$ and $P_1' = \frac{T_1^2 D_{L\uparrow} - T_4^2 D_{L\downarrow}}{T_1^2 D_{L\uparrow} + T_4^2 D_{L\downarrow}}$. Although it looks seemingly like the conventional form, it is clear that the difference of the tunneling amplitudes for the two independent spin channels can still alter the magnitude of the conductance and the polarization as well.

On the other hand, the angular dependence of the tunnel conductance without considering the spin-flip effects, as mentioned before, is well known:

$$G = G_P \cos^2\frac{\theta}{2} + G_{AP} \sin^2\frac{\theta}{2}, \tag{14}$$

with G_P the conductance for parallel orientation of magnetizations in the two FM electrodes, and G_{AP} the conductance for the antiparallel orientation (see e.g. Refs. [1,6]). While in the present case, namely, with inclusion of the effect of spin-flip scatterings we find from Eq.(12) that the angular dependence of the conductance becomes

$$G = G_1 \cos^2\frac{\theta}{2} + G_2 \sin^2\frac{\theta}{2} + G_3 \sin\theta, \tag{15}$$

where $G_1 = \frac{\pi e^2}{2\hbar}\{D_{R\uparrow}[T_1^2 D_{L\uparrow} + T_3^2 D_{L\downarrow}] + D_{R\downarrow}[T_2^2 D_{L\uparrow} + T_4^2 D_{L\downarrow}]\}$, $G_2 = \frac{\pi e^2}{2\hbar}\{D_{R\uparrow}[T_2^2 D_{L\uparrow} + T_4^2 D_{L\downarrow}] + D_{R\downarrow}[T_1^2 D_{L\uparrow} + T_3^2 D_{L\downarrow}]\}$, and $G_3 = \frac{\pi e^2}{2\hbar}(D_{R\uparrow} - D_{R\downarrow})(T_1 T_2 D_{L\uparrow} + T_3 T_4 D_{L\downarrow})$. One may see that apart from the conventional $\cos^2\frac{\theta}{2}$ and $\sin^2\frac{\theta}{2}$ terms there is an additional third term proportional to $\sin\theta$. Here we should point out that G_1 is the conductance in the case of the parallel alignment ($\theta = 0$) for the magnetizations of the two ferromagnets, G_2 is corresponding to the antiparallel case ($\theta = \pi$), and G_3 gives an additional term for the noncollinear case ($\theta \neq 0$ and π), which disappears in the collinear cases. Certainly, these three coefficients G_i ($i = 1, 2, 3$) contain the contributions from the spin-flip scatterings characterized by T_2 and T_3. It is the effect of spin-flip scatterings that enables the tunnel conductance not to be at the minimum when the magnetizations of the two ferromagnets are antiparallel. This is understandable, because the spin-flip scattering process violates the spin conservation and can enable electrons in the spin-up band of one FM electrode tunneling through the insulator barrier into the spin-down band of another FM electrode, and vice versa, thereby giving rise to a phase shift, as shown in Eq.(12). It is emphasized that this shift will disappear when the effect of spin-flip scattering is neglected. Therefore, Eqs. (12) and (15) can be viewd as a generalization of the conventional expression for the tunnel conductance [see Eq.(14)]. It is interesting to note that the phenomenon of such an angular shift has been experimentally observed for a CoFe/Al_2O_3/Co tunnel junction,

as presented in Ref. [8] (see Fig.4 therein), where the maximum of the junction resistance appears at $\theta = 200°$, not $180°$, implying the angular shift $\theta_f = 20°$. Although the authors of Ref. [8] did not mention the reasons why such an angular shift occurs in this FM-I-FM junction, in accordance with the aforementioned analysis we may attribute this phenomenon possibly to the effect of the spin-flip scatterings. If this is acceptable, we can in turn infer the magnitude of the effect of spin-flip scatterings. To show it explicitly, let us assume $T_1 \approx T_4$ and $T_2 \approx T_3$ for simplicity, and define a parameter

$$\gamma = \frac{T_2}{T_1}, \tag{16}$$

which characterizes the magnitude of the effect of spin-flip scatterings. The angular shift θ_f versus the parameter γ is plotted in Fig. 1. It is seen that θ_f is monotonously increasing with increasing γ. When γ approaches to 1, $\theta_f = 90°$ which can be obtained from the expression of P_1 (see below). If $\gamma > 1$, then P_1 can be negative, leading to θ_f larger than $90°$. To see more clearly the effect of spin-flip scatterings on the conductance, we note that G_0 in Eq. (12) can be written as $G_0 = (1+\gamma^2)\bar{G}_0$. In this case, $P_1 = \frac{1-\gamma^2}{1+\gamma^2}\bar{P}_1$, and $P_3 = \frac{2\gamma}{1+\gamma^2}$. The γ-dependence of the conductance is presented in Fig. 2 (a). It can be seen that the conductance decreases with increasing γ when the magnetizations in the two ferromagnets are parallel, while it increases for the antiparallel alignment. As $\gamma > 1$, one may observe that $G(\theta = \pi) > G(\theta = 0)$, suggesting that the inverse TMR may occur. For the case of noncollinear alignments, with increasing γ the conductance first increases rapidly and then decreases, and some peaks appear around $\gamma \approx 1$.

We come to consider the effect of spin-flip scatterings on the TMR. Recently, a number of experiments [4] for a few FM-I-FM tunnel junctions show that if the insulator thin film is the material which differs from Al_2O_3, such as $SrTiO_3$, $Ce_{0.69}La_{0.31}O_{1.845}$ and so on, the TMR, defined as usual as $1 - G(\theta = \pi)/G(\theta = 0)$, will be negative under certain conditions, which means $G(\theta = \pi) > G(\theta = 0)$, exhibiting the so-called inverse TMR effect. It is generally believed that this effect may originate from the electronic states at the interface between a ferromagnetic layer and an insulating layer [4] which could give rise to the density of states in the minority spin band larger than that in the majority spin band at the Fermi level. However, one may see below that the spin-flip scattering can also contribute to the inverse TMR. From (12) we find that the TMR still has the apparently standard form

$$TMR = \frac{2P_1P_2}{1 + P_1P_2}, \tag{17}$$

but P_1, defined after Eq. (12) and containing the contribution from spin-flip scatterings, differs from the conventional polarization $\bar{P}_1$. In Ref. [3], Moodera et al calculated the TMR for the $CoFe/Al_2O_3/Co$ junction according to the Jullière's formula. The calculated result is 27%, while the experiment value is 24% at 4.2 K. If we adopt this experimental data, we can calculate the contribution of the spin-flip scatterings which is characterized by the parameter γ. The obtained result for γ is about 0.28, where the spin polarization of electrons is taken as 47% for CoFe and 34% for Co [3]. It shows that the spin-flip scatterings might have a considerable effect on the electrical transport of this tunnel junction. On the other hand, if we take the contribution from the spin-flip scatterings into account, then we can apply our formula to estimate the value of TMR, which could be closer to the experimental result

than using Jullière′s formula. If the tunneling amplitudes satisfy a certain condition, P_1 can be negative, depending on the difference between $(T_1^2 - T_2^2)D_{L\uparrow}$ and $(T_4^2 - T_3^2)D_{L\downarrow}$, resulting in that the TMR can be negative. The γ-dependence of the TMR is depicted in Fig. 2 (b). It can be seen that the TMR decreases with increasing γ, and becomes negative for $\gamma > 1$. This can be understood in the following. For $0 < \gamma < 1$, the tunneling amplitude for the two independent channels (T_1) is larger than the tunneling amplitude for the spin-flip channel (T_2). Owing to the spin-flip scatterings the polarization P_1 becomes effective and small, leading to decreasing of the TMR. When $\gamma > 1$, i.e., the tunneling amplitude for the two independent channels is smaller than that for the spin-flip channel, the spin-flip scattering dominates in the tunneling process, implying that the electrons with spin up in the left FM electrode can tunnel through the insulator barrier to occupy the states of electrons with spin down in the right FM electrode via the spin-flip mechanism, thereby giving rise to contribution to the inverse TMR effect.

The angular dependence of the TMR can be understood from the following definition

$$TMR(\theta) = \frac{G(\theta) - G(\theta = \pi)}{G(\theta = 0)} = \frac{P_2(P_1 + \sqrt{P_1^2 + P_3^2}\cos(\theta - \theta_f))}{1 + P_1 P_2}. \tag{18}$$

When $\theta = \theta_f$, the TMR goes to its maximum which will be denoted by $TMR(\theta_f)$ hereafter. In Fig. 3, the γ-dependence of the maximum TMR, i.e. $TMR(\theta_f)$, is presented. A remarkable property is that $TMR(\theta_f)$ has a peak at $\gamma \approx 0.82$, which migh be a result of the spin-flip assisted tunneling. It is seen that $TMR(\theta_f)$ approaches to a constant when γ increases to a large value. No matter how large γ is, $TMR(\theta_f)$ is always positive.

The above discussion is based on the result up to the first-order approximation for the Green functions. To include contributions from higher-order Green functions, it is better to consider them in a Keldysh space. We introduce the nonequilibrium Green function in the Keldysh space as [9]

$$\widehat{\mathbf{G}}_{qk}(t,\ t') = \begin{pmatrix} \mathbf{G}^t_{qk}(t,\ t') & \mathbf{G}^<_{kq}(t,\ t') \\ \mathbf{G}^>_{qk}(t,\ t') & \mathbf{G}^{\tilde{t}}_{qk}(t,\ t') \end{pmatrix}, \tag{19}$$

where $\mathbf{G}^t_{qk}(t,\ t')$ is the time-ordered Green function defined as before, $\mathbf{G}^{<(>)}_{kq}(t,\ t')$ is lesser (greater) Green function, and $\mathbf{G}^{\tilde{t}}_{qk}(t, t')$ is the antitime-ordered Green function. The elements of $\mathbf{G}^{\tilde{t}}_{qk}(t,\ t')$ and $\mathbf{G}^>_{qk}(t,\ t')$ are given by

$$\begin{aligned} G^{\sigma\sigma',\tilde{t}}_{qk}(t,\ t') &= -i\langle \widetilde{T}[b_{q\sigma}(t)a^\dagger_{k\sigma'}(t')]\rangle, \\ G^{\sigma\sigma',>}_{kq}(t,\ t') &= -i\left\langle b_{q\sigma}(t)a^\dagger_{k\sigma'}(t')\right\rangle. \end{aligned} \tag{20}$$

According to Eqs. (5) and (6), we can make a sum of Feynman diagrams shown in Fig. 4. The result is

$$\widehat{\mathbf{G}}_{kq}(\varepsilon) = \widehat{\mathbf{g}}_R(\varepsilon)\widehat{\mathbf{\Sigma}}(\varepsilon)\widehat{\mathbf{g}}_L(\varepsilon), \tag{21}$$

where $-i\widehat{\mathbf{\Sigma}}(\varepsilon) = -i\Omega^\dagger\widehat{\tau}_3(\widehat{1} - \widehat{\eta})^{-1}$, $\widehat{\eta} = \widehat{\mathbf{g}}_L(\varepsilon)\Omega\widehat{\tau}_3\widehat{\mathbf{g}}_R(\varepsilon)\Omega^\dagger\widehat{\tau}_3$, $\mathbf{\Omega} = \mathbf{T}\cdot\mathbf{R}$, and $\widehat{\tau}_3$ is a Pauli matrix. From Eq. (2), the current can be rewritten as

$$I_L(V) = -\frac{2e}{\hbar}\,\mathrm{Re}\int \frac{d\varepsilon}{2\pi} Tr_\sigma\{(\mathbf{\Omega}\widehat{\mathbf{G}}_{qk}(\varepsilon))_{12}\}. \tag{22}$$

After a tedious calculation, we get

$$\begin{aligned} I_L(V) = -\frac{e}{\hbar}\,\mathrm{Re}\int \frac{d\varepsilon}{2\pi} Tr\{&\widehat{\mathbf{F}}_2(\widehat{\tau}_3 - i\widehat{\tau}_2)\widehat{\mathbf{F}}_1\mathbf{T}_{eff}(\varepsilon,V)[(1+\mathbf{T}_{eff}(\varepsilon,V)/2)\widehat{\tau}_0 \\ &+(f(\varepsilon+eV)-f(\varepsilon))(\widehat{\tau}_3 + i\widehat{\tau}_2)\mathbf{T}_{eff}(\varepsilon,V)]^{-1}\}, \end{aligned} \tag{23}$$

where Tr denotes the trace over the spin space and the Keldysh space, $\widehat{\tau}_0$ is the unit matrix, $\widehat{\tau}_i$ $(i=1,2,3)$ are Pauli matrices, and

$$\widehat{\mathbf{F}}_1 = \begin{pmatrix} 1-2f(\varepsilon) & 0 \\ 0 & 2f(\varepsilon) \end{pmatrix};\ \widehat{\mathbf{F}}_2 = \begin{pmatrix} 2f(\varepsilon+eV) & 0 \\ 0 & 1-2f(\varepsilon+eV) \end{pmatrix}.$$

Eq. (23) can be rewritten in a compact form

$$I_L(V) = \frac{4e}{h}\,\mathrm{Re}\int d\varepsilon[f(\varepsilon+eV)-f(\varepsilon)]Tr_\sigma\{[\mathbf{\Lambda}(\varepsilon,V)-1]\cdot\mathbf{\Lambda}(\varepsilon,V)\}, \tag{24}$$

where $\mathbf{\Lambda}(\varepsilon,V) = \frac{\mathbf{T}_{eff}(\varepsilon,V)}{2}\cdot(1+\frac{\mathbf{T}_{eff}(\varepsilon,V)}{2})^{-1}$ and $\mathbf{T}_{eff}(\varepsilon,V) = \begin{pmatrix} T^1_{eff}(\varepsilon,V) & T^2_{eff}(\varepsilon,V) \\ T^3_{eff}(\varepsilon,V) & T^4_{eff}(\varepsilon,V) \end{pmatrix}$ are matrices in spin space, and $T^i_{eff}(i=1,2,3,4)$ are the elements of the effective transmission matrix $\mathbf{T}_{eff}(\varepsilon,V)$ given in Eq. (10). In principle, Eq. (24) gives the current including more corrections from the spin-flip scatterings, and the tunnel conductance can be obtained by $G=\partial I_L(V)/\partial V$. For a small bias voltage, we get

$$G = \frac{2e^2}{h}\tilde{T}_{eff}, \tag{25}$$

where $\tilde{T}_{eff} = \frac{[8T^0_{eff}+(T^1_{eff}(\varepsilon_F)+T^4_{eff}(\varepsilon_F))(2+T^0_{eff})]}{[2+T^0_{eff}+(T^1_{eff}(\varepsilon_F)+T^4_{eff}(\varepsilon_F))]^2}$ with $T^0_{eff} = 2\pi^4 D_{L\uparrow}(\varepsilon_F)D_{L\downarrow}(\varepsilon_F)D_{R\uparrow}(\varepsilon_F)D_{R\downarrow}(\varepsilon_F)(T_1T_4 - T_2T_3)^2$, can be viewed as the effective transmission coefficient. Compared to Eq. (11), Eq. (25) includes more corrections from the spin-flip scatterings. Although the angular dependence of $G(\theta)$ determined by Eq. (25) looks more complex in form than one presented in Eq. (12), the behavior of $G(\theta)$ versus θ is found to be qualitatively similar to those shown in Fig. 2 (a) for a given γ.

In summary, we have investigated the effect of spin-flip scatterings on the spin-dependent electrical transport in ferromagnet-insulator-ferromagnet tunnel junctions by using the nonequilibrium Green function technique. When the effect of the spin-flip scatterings is taken into account, the frequently used Jullière′s formula for the tunnel conductance must be modified, though the form looks seemingly similar. It is found that the spin-flip scatterings could lead to an angular shift of the tunnel conductance, giving rise to the junction resistance not being the largest when the orientations of magnetizations in the two FM electrodes are antiparallel, which is quite consistent with the experimental observation in CoFe/Al_2O_3/Co tunnel junctions. As the Jullière′s formula overestimates the value of the TMR, our derived formula with inclusion of the effect of spin-flip scatterings could estimate the TMR value closer to the experimental result, as discussed above. It is found that the spin-flip scattering could also lead to the inverse TMR effect under certain conditions,

though it is not the only factor. The phenomenon of spin-flip assisted tunneling is clearly observed. When including high-order terms of the Green function, the angular dependence of the tunnel conductance is qualitatively similar, although the form looks more complex. Finally, we would like to mention that our present derivation can be readily extended to other magnetic junctions.

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FIGURE CAPTIONS

Fig. 1 The angular shift θ_f versus the parameter γ, where the mass of single electron in both ferromagnets are assumed as unity, the molecular fields in the two ferromagnets are supposed to be the same and taken as $0.7eV$, $\varepsilon_F = 1.5eV$, and the coupling parameter T_1 is chosen as 0.01 eV.

Fig. 2 The γ-dependence of the tunnel conductance (a) and the TMR (b), where the parameters are taken the same as those in Fig. 1.

Fig. 3 The γ-dependence of the maximum tunnel magnetoresistance $TMR(\theta_f)$, where the parameters are taken the same as those in Fig. 1.

Fig. 4 Feynman diagrams for the Green function $\widehat{\mathbf{G}}_{qk}(\varepsilon)$.

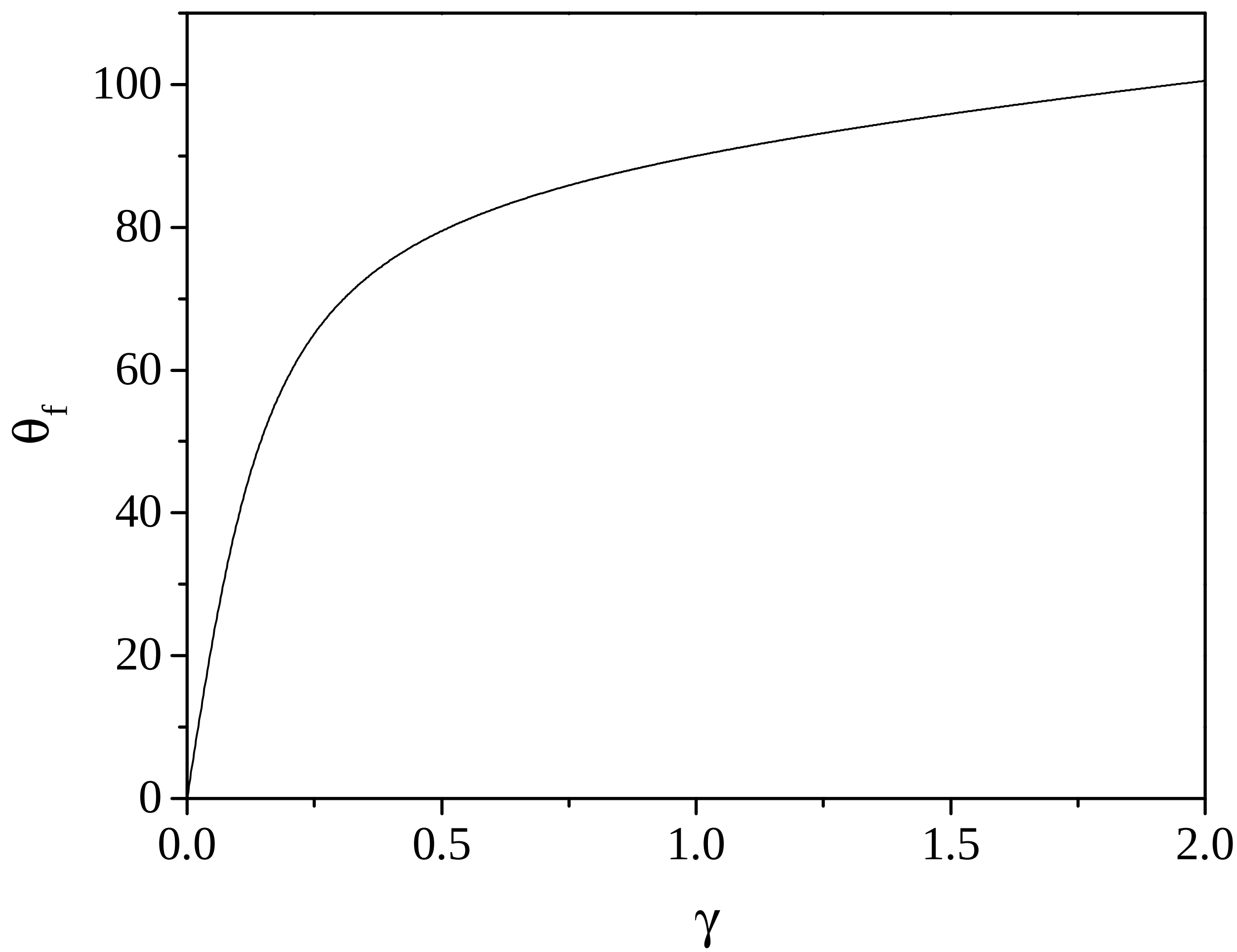

Fig.1 Zhu et al

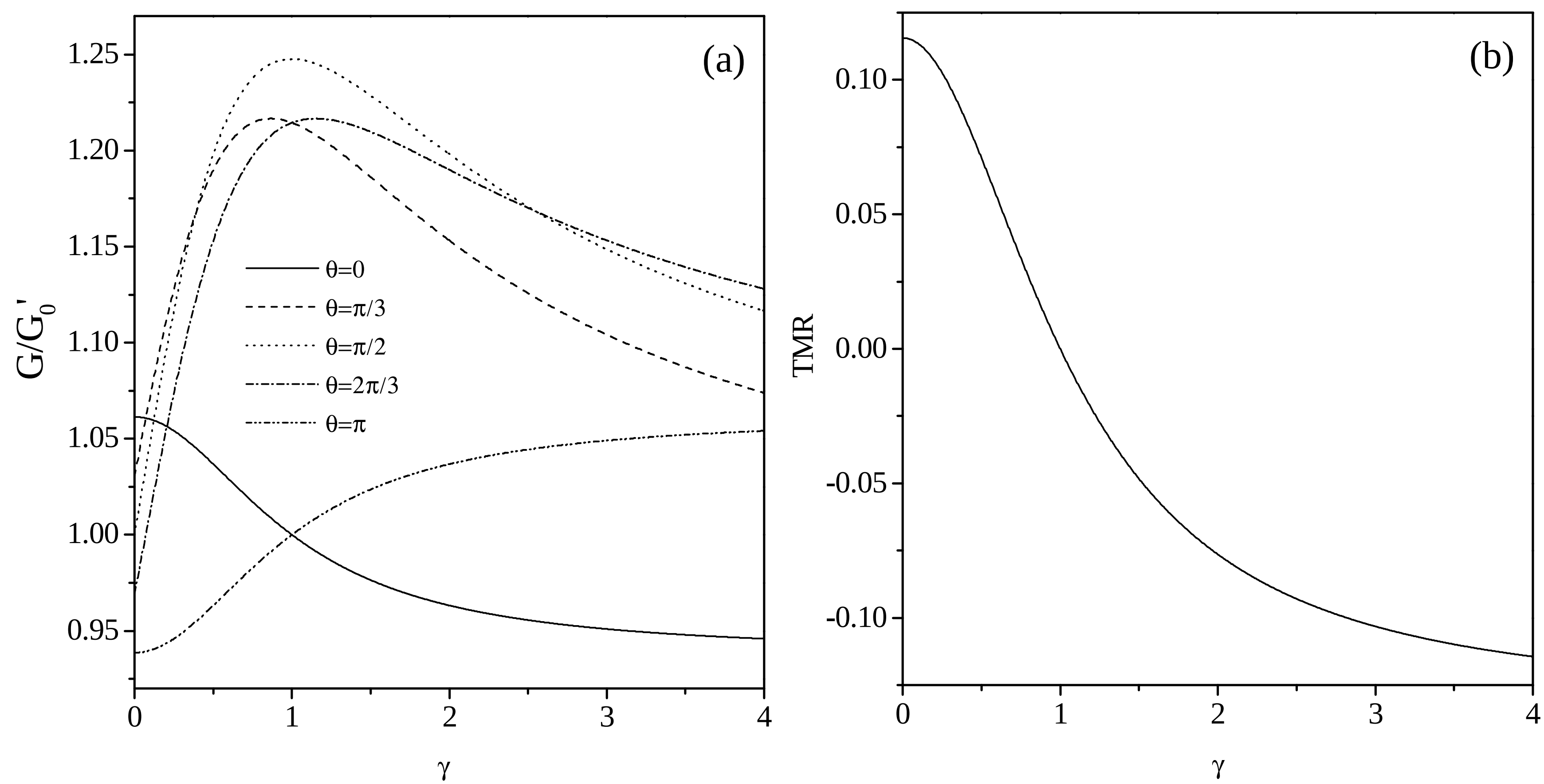

Fig.2 Zhu et al

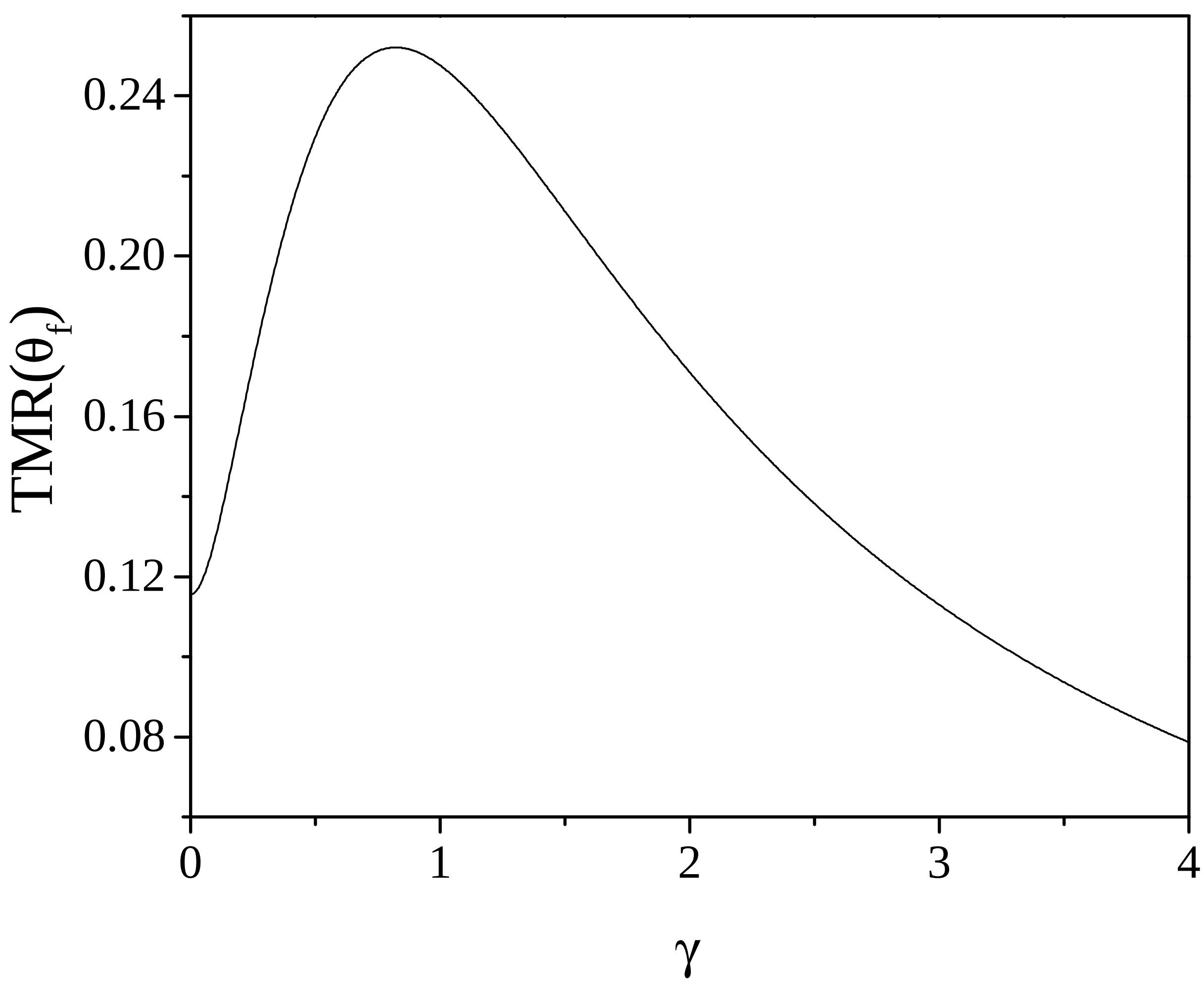

Fig.3 Zhu et al

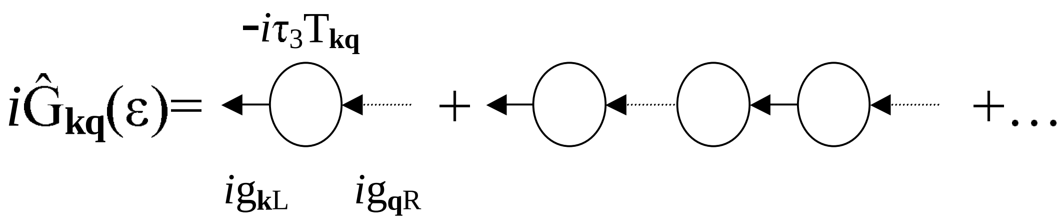

Fig.4 Zhu et al